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Title: Effects of Line Shifts and the Ion Quadrupole Contribution on Spectral Line Assymetries

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Effects of Line Shifts and the Ion Quadrupole Contribution on Spectral Line Asymmetries

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Acknowledgements

Charles F. Hooper (1932-2002)

In my opinion, Professor Hooper was probably one of the best professors in the physics department at the University of Florida in that he always treated his graduate students with respect and was always willing to listen to and help his students in any way possible. This is probably why so many of his former students currently have very successful careers. Most of the research and results presented in this poster is the culmination of 35 years of work by Professor Hooper's research group in using spectral line emission from plasmas as a diagnostic of plasma conditions.

Further information can be found at: www.phys.ufl.edu/hooper.html

Acknowledgements

Gwyneth C. Junkel-Vives (1964-2001)

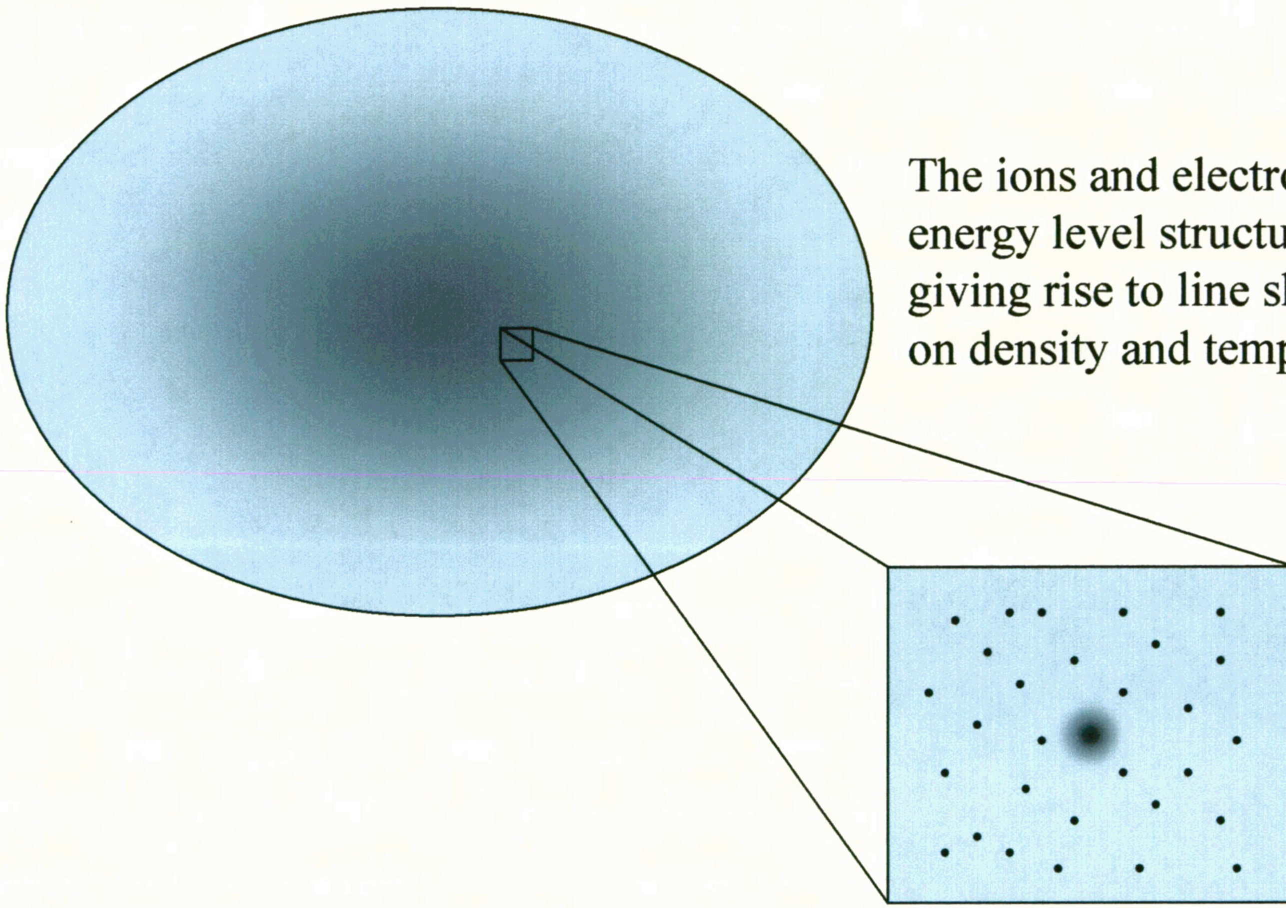
Gwyneth and I were graduate students in Professor Hooper's research group, and we worked closely on various research projects during latter portion of the 1990s. After graduating in June of 2000, she came to work as a postdoc at Los Alamos National Laboratory and had a very successful postdoctoral research experience. A significant portion of the results shown in this presentation is based on the research work that she did as a graduate student.

Introduction and Outline

Line asymmetries and the corresponding shift of spectral lines due to the electron penetration of the radiator orbitals and the ion quadrupole contribution become more significant with increasing principal quantum number and increasing electron density.

- The mean field static shift due to electron penetration of the orbitals gives rise to an overall shift of the line to lower energy and a significant asymmetry near line center, but does not generate much red/blue far wing asymmetry.
- The ion quadrupole contribution results in a small blue shift of the spectral line and a small change in asymmetry near line center, but it gives rise to a significant red/blue wing asymmetry in the far wings of the line.
- Experimental data from recent spherical implosion experiments on OMEGA shows evidence of the mean field static shift and may also show the effects of level interactions between the Ar Lyman -γ, -δ, -ε lines and also the Ar He -γ, -δ lines.

The plasma is broken into cells, each cell containing one charged radiator with many perturbing ions and electrons



The ions and electrons perturb the energy level structure of the radiator, giving rise to line shapes dependent on density and temperature.

The radiator-ion and radiator-electron interactions of the plasma Hamiltonian are broken into a monopole term and a remainder.

Electron-radiator interaction excluding the monopole term

$$H' = H_r^0 + \left(H_i^0 + V_{i,r}^0 + V_{i,e}\right) + \left(H_e^0 + V_{e,r}^0\right) + V_{e,r}^1 + V_{i,r}^1$$

Monopole terms

$$V_{i,r}^1\left(\vec{E}\right) = \vec{d}\cdot\vec{E} + \frac{1}{4}Q_{zz}\langle E_{zz}\rangle_E$$

Ion field or Stark splitting

The electron-radiator interaction without the monopole term consists of an internal structure term and the higher order poles.

$$V_{1e,r}^{1} = e^{2}\sum_{i=1}^{N_r}\sum_{t=0}^{\infty}\sum_{q=-t}^{t} A^{t}(r_i, r_{1e})C_q^{(t)}(\theta_i, \varphi_i)C_q^{(t)*}(\theta_{1e}, \varphi_{1e})$$

$$A^{t}(r_i, r_{1e}) = \left(\frac{r_<^{t}}{r_>^{t+1}} - \frac{\delta_{t,0}}{r_{1e}}\right)$$

t = 0 gives a monopole-like orbital penetration term

$$C_q^{(t)}(\theta, \varphi) = \left(\frac{4\pi}{2t+1}\right)^{\frac{1}{2}} Y_{tq}(\theta, \varphi)$$

In pressure broadening theory, we can state the line shape function as an average over possible values of the ion microfield.

$$I(\omega) = \frac{1}{\pi} \Re \int_0^\infty dt\, e^{i(\omega - i\varepsilon)t} \mathrm{Tr}\left\{ \vec{d} \cdot e^{\frac{-iH't}{\hbar}} \rho \vec{d} e^{\frac{iH't}{\hbar}} \right\}$$

Lineshape

$$= \underbrace{\int_0^\infty d\vec{E}\, Q(\vec{E})}_{} \boxed{J(\omega, \vec{E})}$$

Average weighted by ion microfield distribution function

Electron-broadened lineshape emitted by a radiator experiencing a ion microfield ***E***

$$Q(\vec{E}) = \mathrm{Tr}_i \left\{ \rho_i \delta\left(\vec{E} - \vec{E}_{si}\right) \right\}$$

- The effects of the motion of the radiator on the line shape are included by convolving this expression with a gaussian shaped Doppler profile.

The field dependent line shape function has three important contributions: Ion dynamics, Stark splitting, and electron broadening effects.

$$J(\omega,\vec{E}) = -\frac{1}{\pi}\,\mathrm{Im}\,\mathrm{Tr}_r\left\{\vec{\mathrm{d}}\cdot G(\omega,\vec{E})\frac{1}{1-\upsilon\underbrace{\int d\vec{E}'Q(\vec{E}')G(\omega,\vec{E}')}_{\text{Ion dynamics effects}}}f_r\,\vec{\mathrm{d}}\right\}$$

$$G(\omega,\vec{E}) = \frac{1}{\Delta\omega - V_{ir}^{1}(\vec{E}) - \boxed{M'(\omega)} - i\upsilon}$$

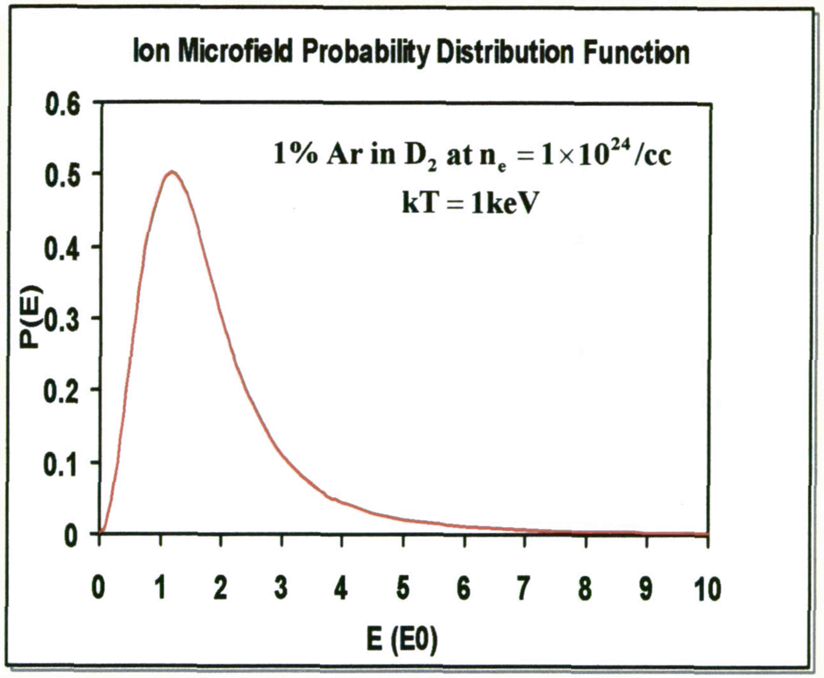
Ion dynamics effects

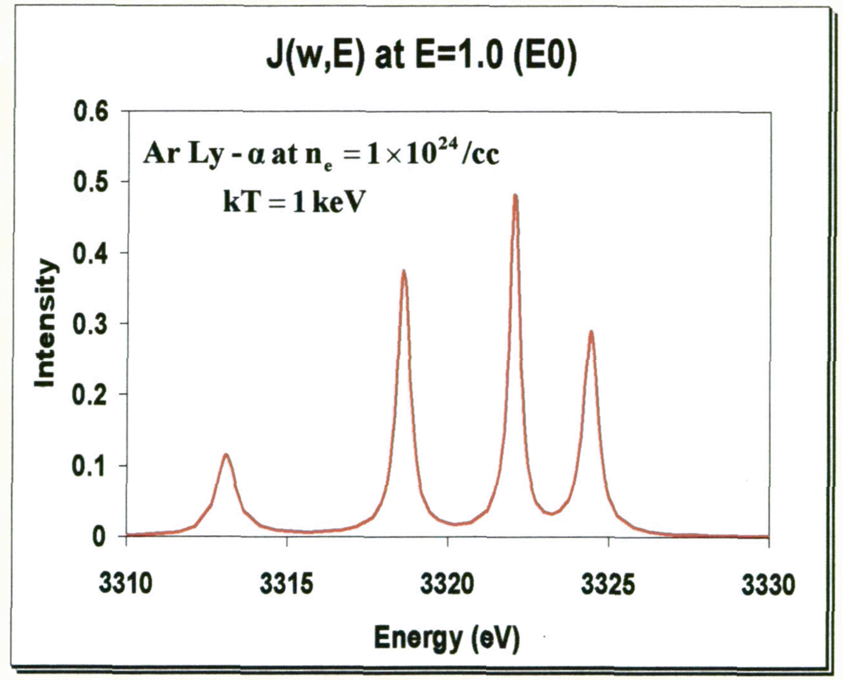
Ion microfield or Stark splitting

Effects of plasma electron-radiator interactions

$$\Delta\omega = \omega - \left(\frac{H_r^{0,\,\text{initial}} - H_r^{0,\,\text{final}}}{\hbar}\right)$$

We provide here an example of what $P(E) = 4\pi E^2 Q(E)$ and $J(\omega, E)$ look like when plotted out.





$$E_0 = \frac{e}{r_{0,e}^2} \quad \text{where} \quad \frac{4}{3}\pi r_{0,e}^3 n_e = 1$$

The width-shift operator to all-order in the electron radiator interaction $V_{1e,r}$ can be converted to 2nd-order with three changes.

Mean field static shift term gives rise to significant shifts due to electron orbital penetration term

Reduced distribution function includes electron-radiator interaction

$$M'(\omega) = n_e \, \mathrm{Tr}_{1e} \left\{ V^1_{1e,r} \boxed{f_{1e,r}} + V^1_{1e,r} \frac{1}{\Delta\omega - H^0_{1e} - \boxed{V^1_{1e,r}}} \boxed{f_{1e,r}} V^1_{1e,r} \right\} f_r^{-1}$$

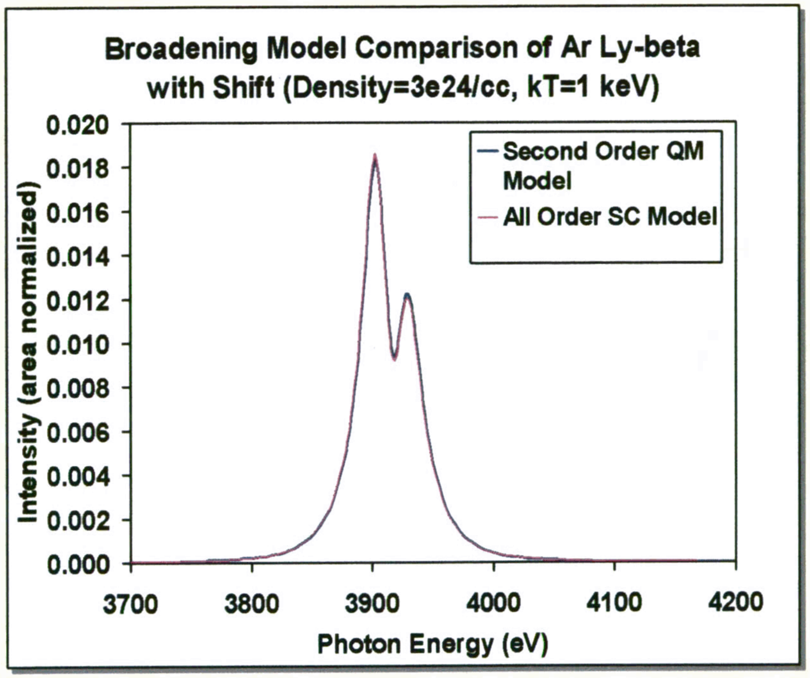
Quantum mechanical (QM) or semiclassical (SC)

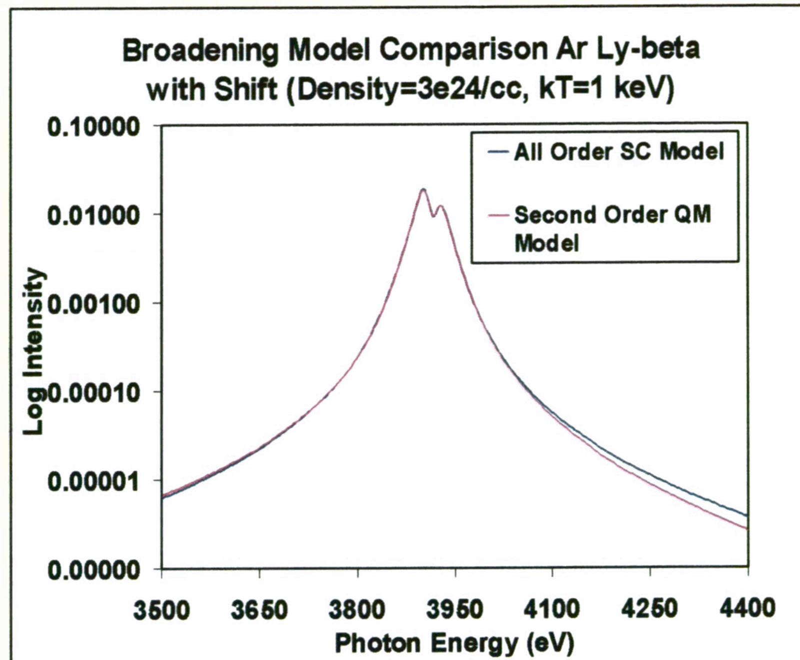
2nd-order : Expand to first order the interaction

2nd-order : Drop this term

2nd-order : Drop dependence on the interaction

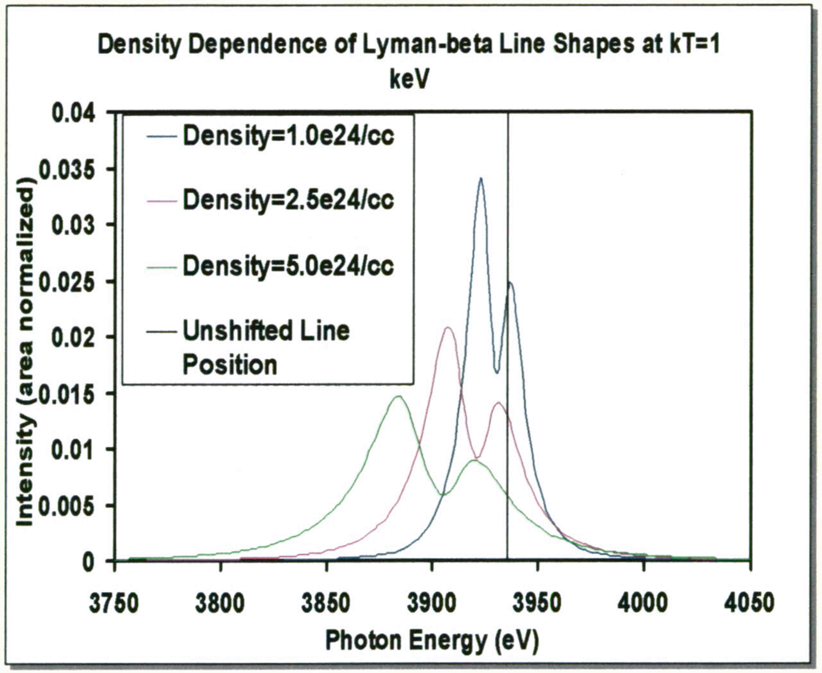
The difference observed in the blue wing arises mainly from the principal value solution of the 2nd-order version of $M'(\omega)$.

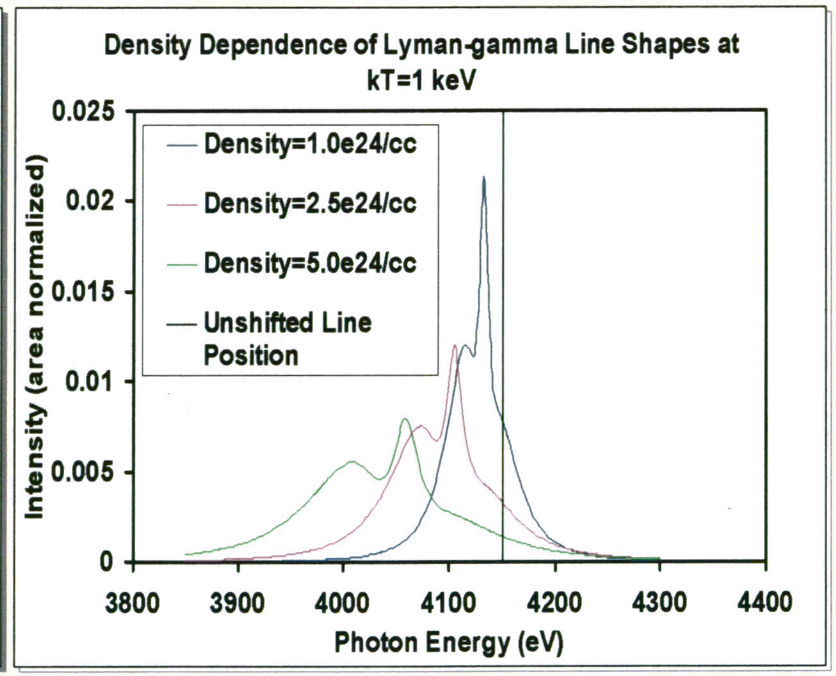




- Due to the properties of the principal value solution to the second order version of the width and shift operator, the width in the blue wing is smaller than it should be, giving rise to the difference.
- All line shapes through the rest of the talk are from argon radiators.

As electron density increases, the line shapes shift to lower energy due to the electron penetration of the orbitals.

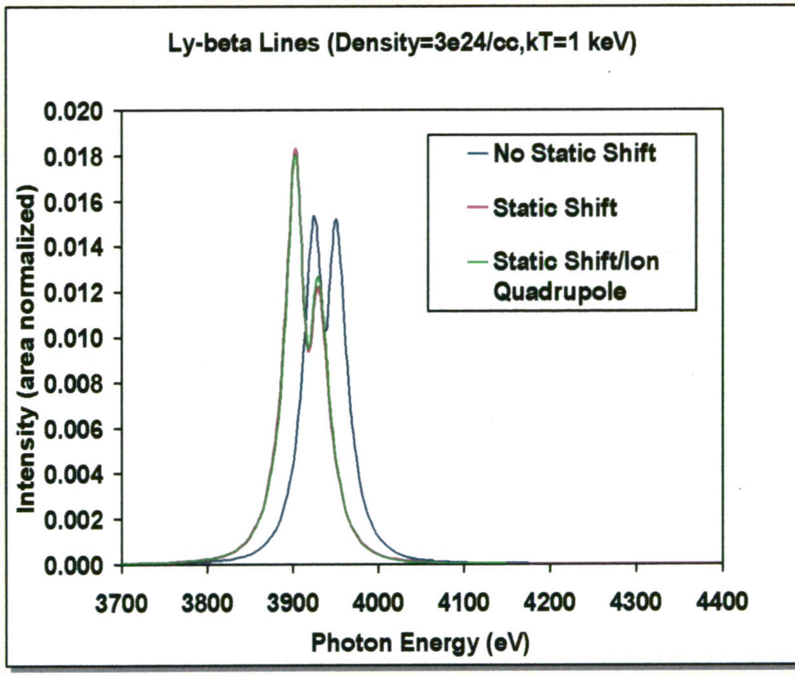


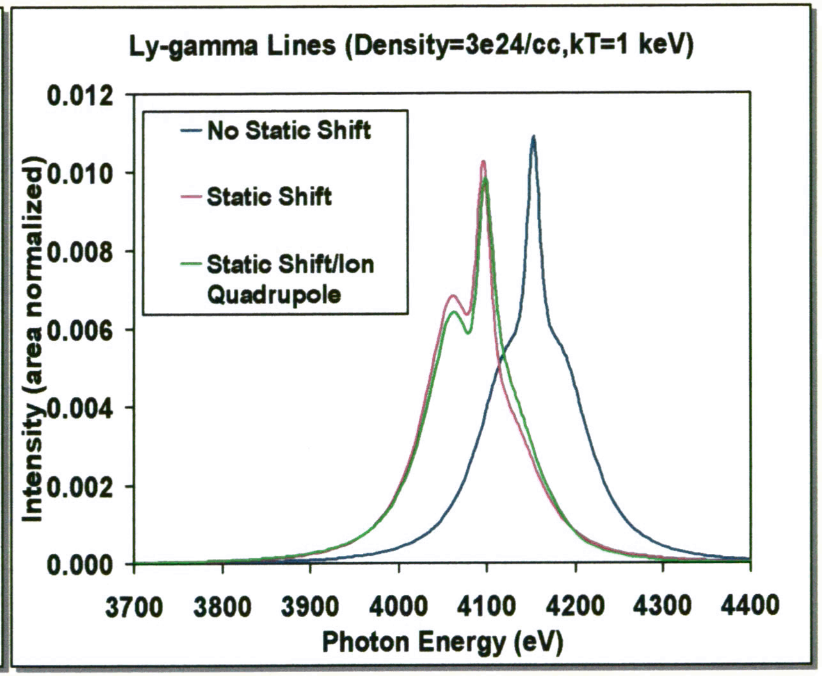


kT=1 keV

- With sufficiently large electron density, the penetrating electrons can effectively shield the nuclear charge from the radiating electron, thus lowering its energy state and resulting in a shift of the spectral line to lower energy.

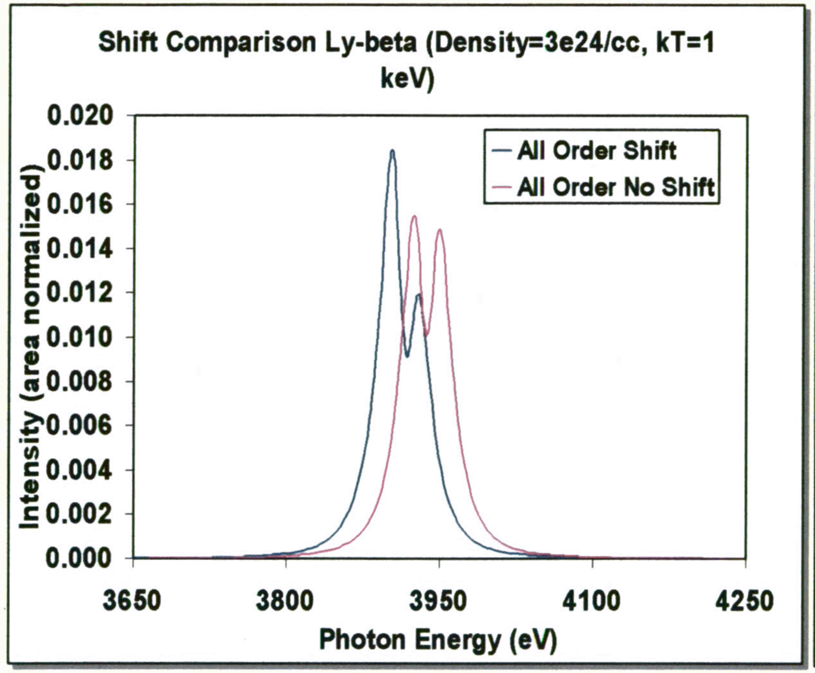
Spectral line shape positions and asymmetries are affected by both the static line shift and the ion quadrupole.

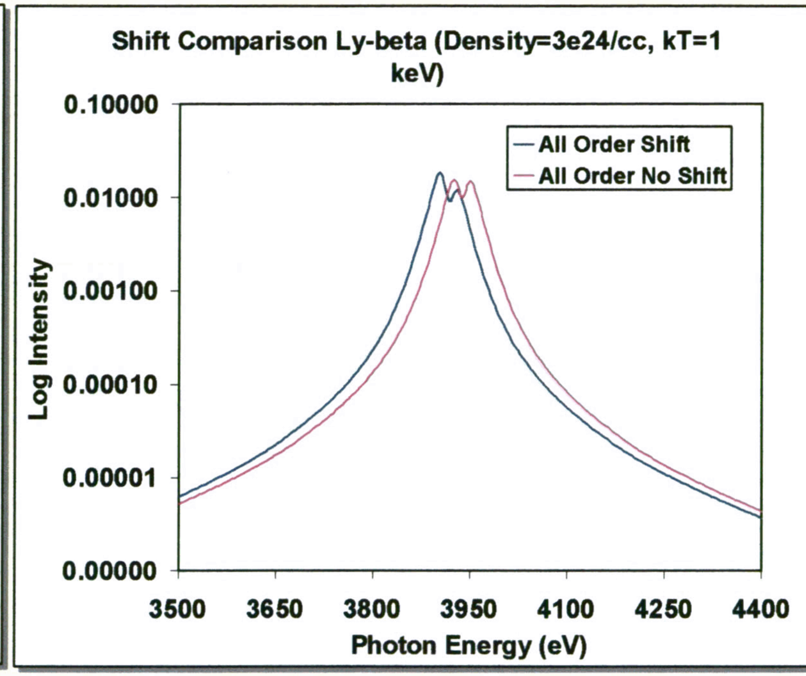




- Note that the effect of the ion quadrupole becomes more significant as the principal quantum number of the spectral line increases. It also becomes somewhat more significant as the electron density increases.

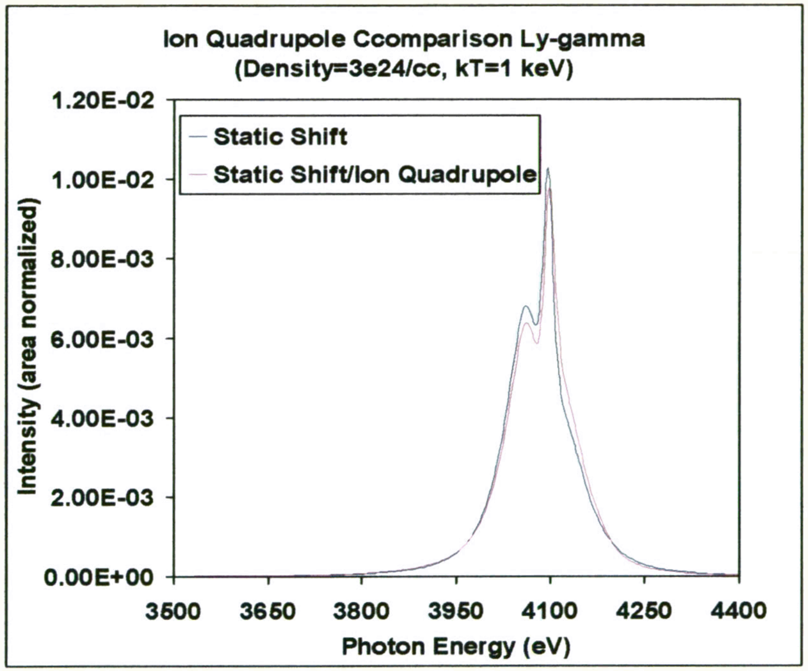
In addition to the overall red shift in the line shapes, the static shift term also causes asymmetry mainly near the line center.

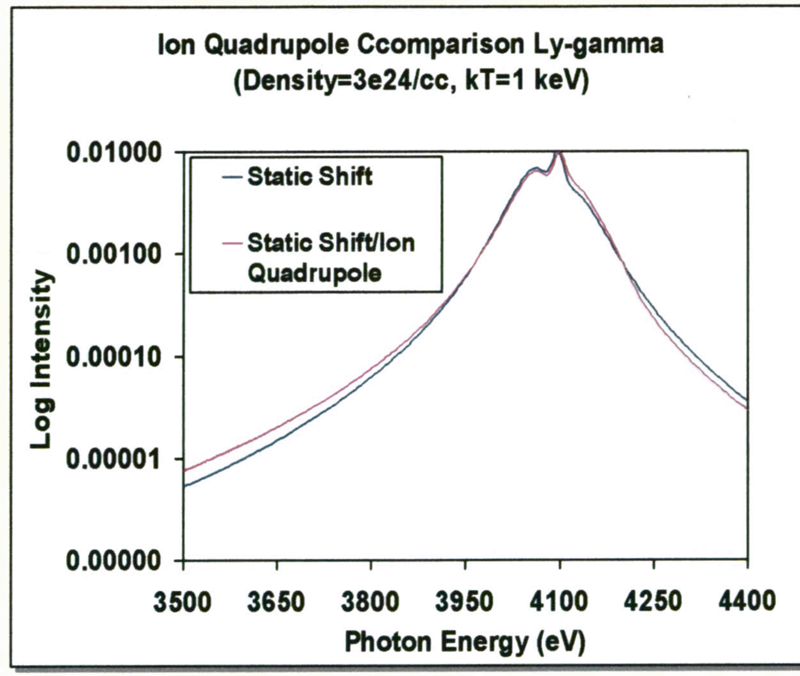




- Note that there does not seem to be much red/blue wing asymmetry in the line shape due to the static shift term.

In addition to shifting the line center to higher energy, the ion quadrupole also significantly alters the wings of the line.





Static Line Shift and Ion Quadrupole Effect

- Note that the effect of the ion quadrupole gives rise to a significant red/blue wing asymmetry in this line shape.

Two hydrodynamics codes were used to simulate spherical implosions experiments performed on the OMEGA laser.

RAGE

- 3D Eulerian code with AMR
- Uses the SESAME EOS tables
- Ionization information derived from SESAME opacity tables (LTE)
- Thermal conduction treated through a diffusion approximation
- Radiation transport limited to non-equilibrium single group (grey) diffusion treatment
- Laser deposition information is taken from a HYADES run and used as an external energy source in a RAGE.

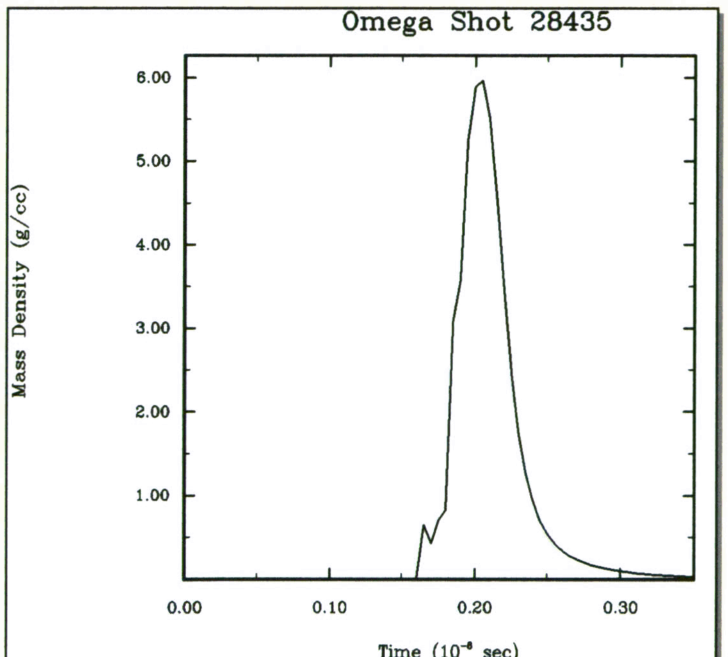
HYADES

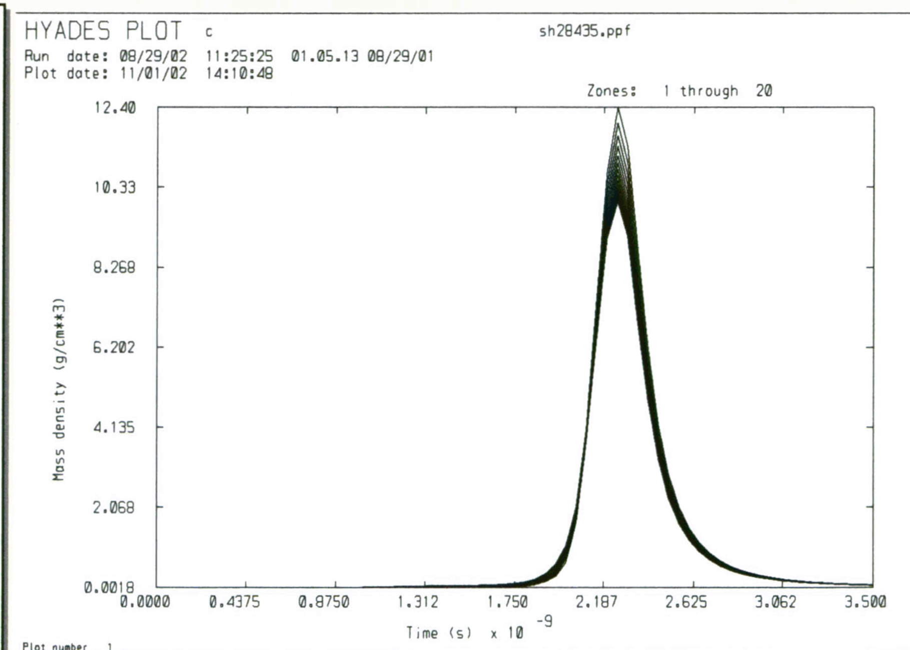
- 1D Lagrangian hydrodynamics code
- Uses EOS tables based on the SESAME EOS tables
- Use average atom LTE ionization model (NLTE model not working)
- Thermal conduction treated through a diffusion approximation
- Radiation transport treated by either non-equilibrium single group (grey) or multi-group diffusion methods

RAGE and HYADES Simulations of Mass Density for Omega Shot 28435

Omega Shot 28435 Specs

- Plastic shell of outer diameter 918.5 microns and shell thickness of 26.3 microns
- Filled with a gas mixture of 0.054 atm Ar in 10 atm DD
- 21.4 KJ on target in a 1 ns square pulse shape





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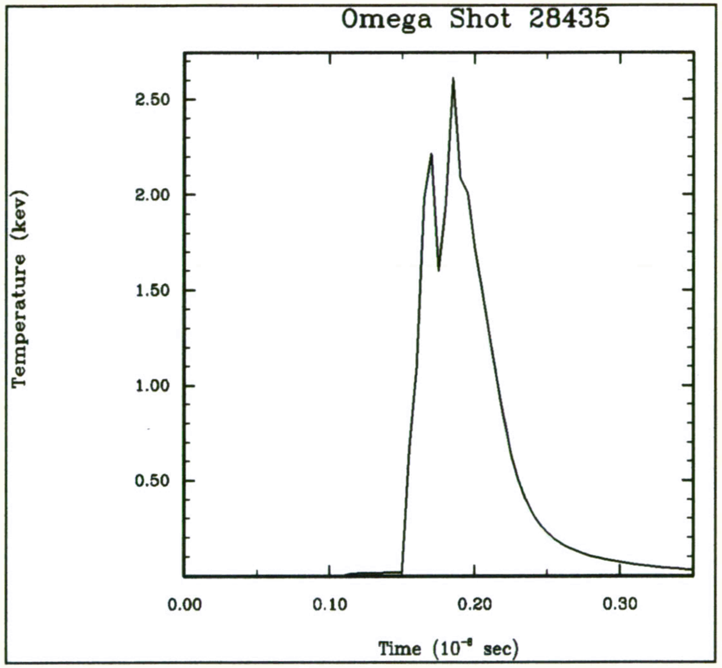
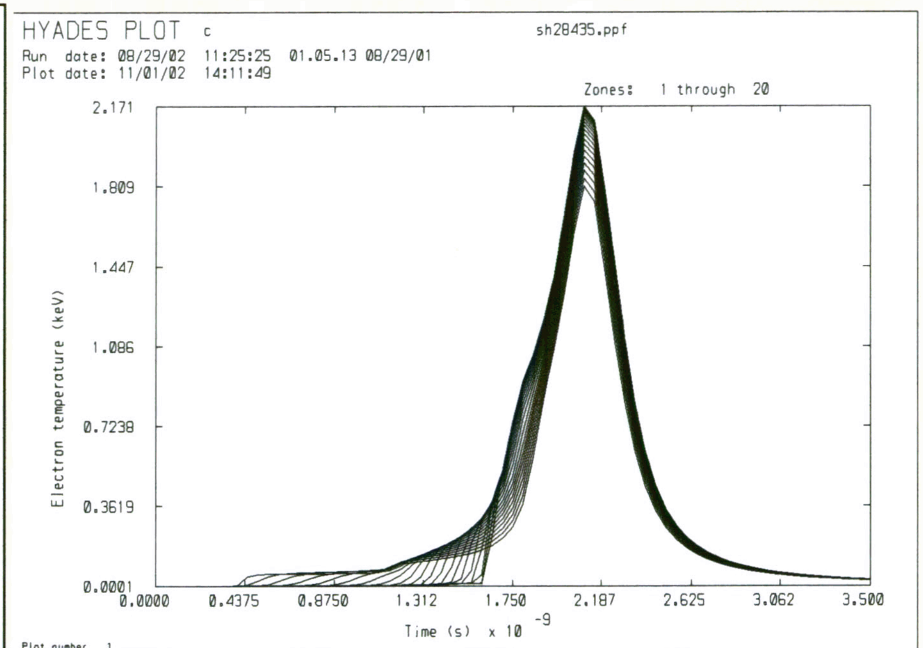
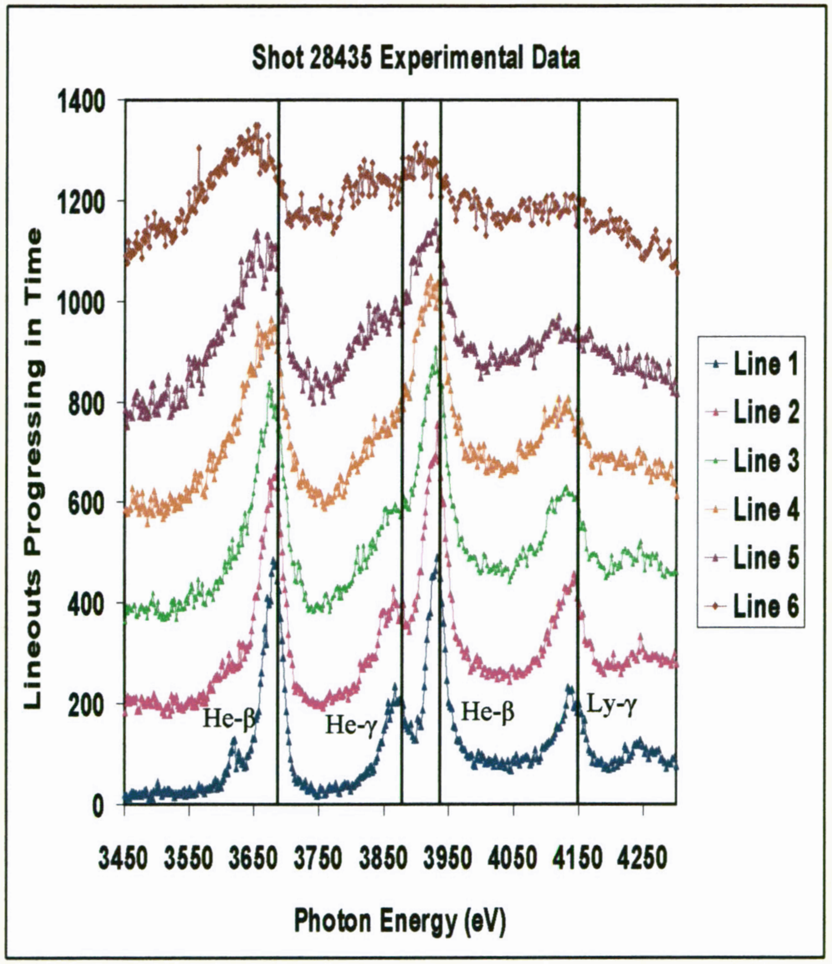
RAGE and HYADES Simulations of Electron Temperature for Omega Shot 28435





- HYADES, with its thermonuclear burn package, predicts a neutron yield of 8.66×10^{10}.

The experimental data from shot 28435 shows a definite shifting of the lines as the implosion progresses.

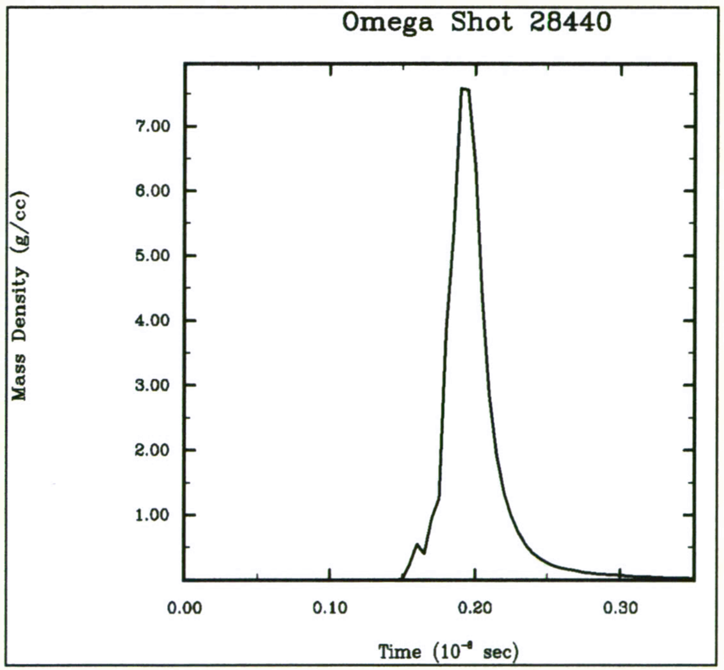


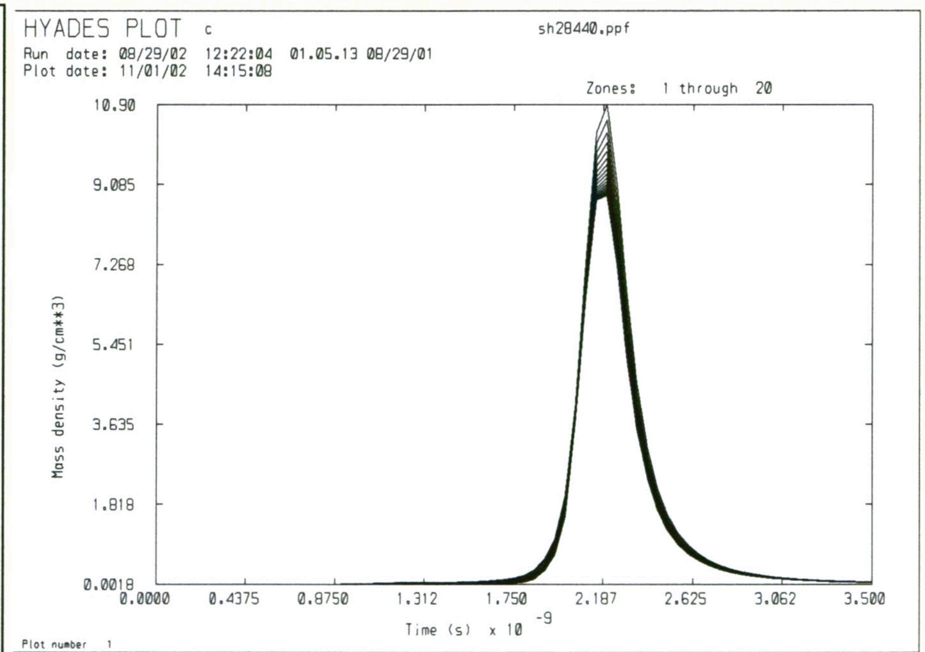
- For every 1×10^{24} electrons/cc, the Ly-β line will shift to the red by about 7.5 eV and the Ly-γ line will shift to the red by about 23 eV as predicted by theory.
- Using the theoretical predictions of how much the lines will shift, the density achieved in this implosion is around 3×10^{24} electrons/cc, or about 5 g/cc, before spectral line become unobservable.
- The neutron yield from this shot was 7.78×10^{9}, and the bang time from the Neutron data was 2.15 ns.

RAGE and HYADES Simulations of Mass Density for Omega Shot 28440

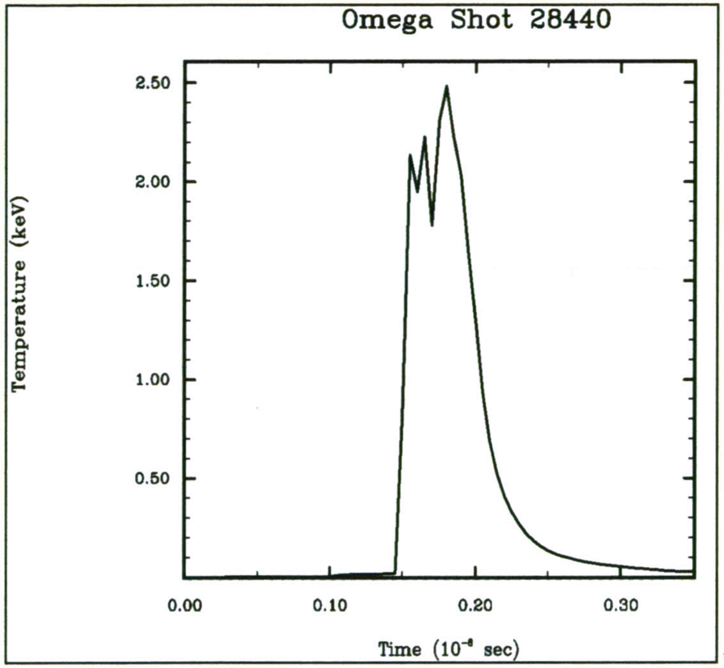
Omega Shot 28440 Specs

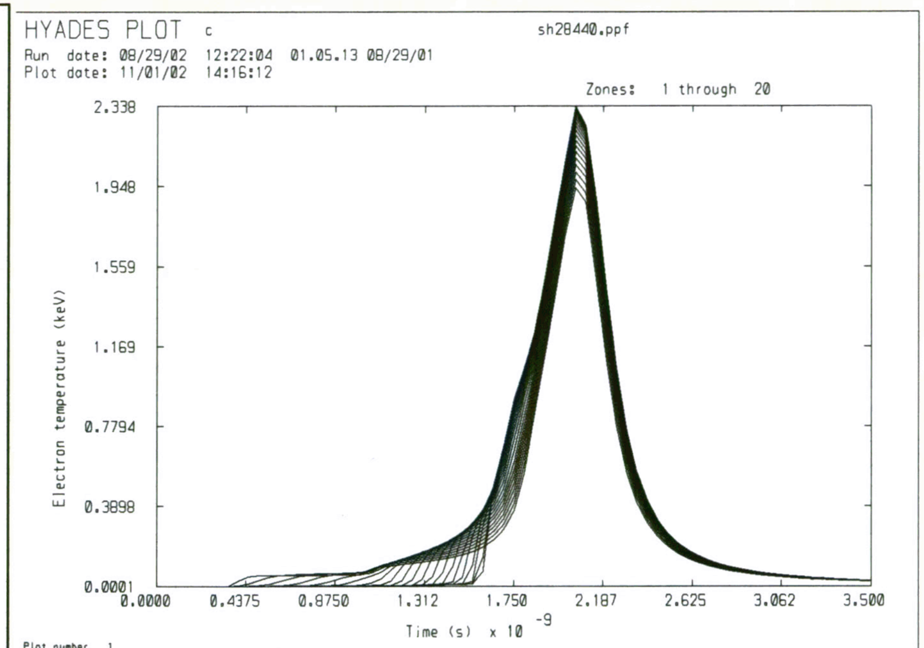
- Plastic shell of outer diameter 949 microns and shell thickness of 23.5 microns
- Filled with a gas mixture of 0.054 atm Ar in 10 atm DD
- 21.8 KJ on target in a 1 ns square pulse shape





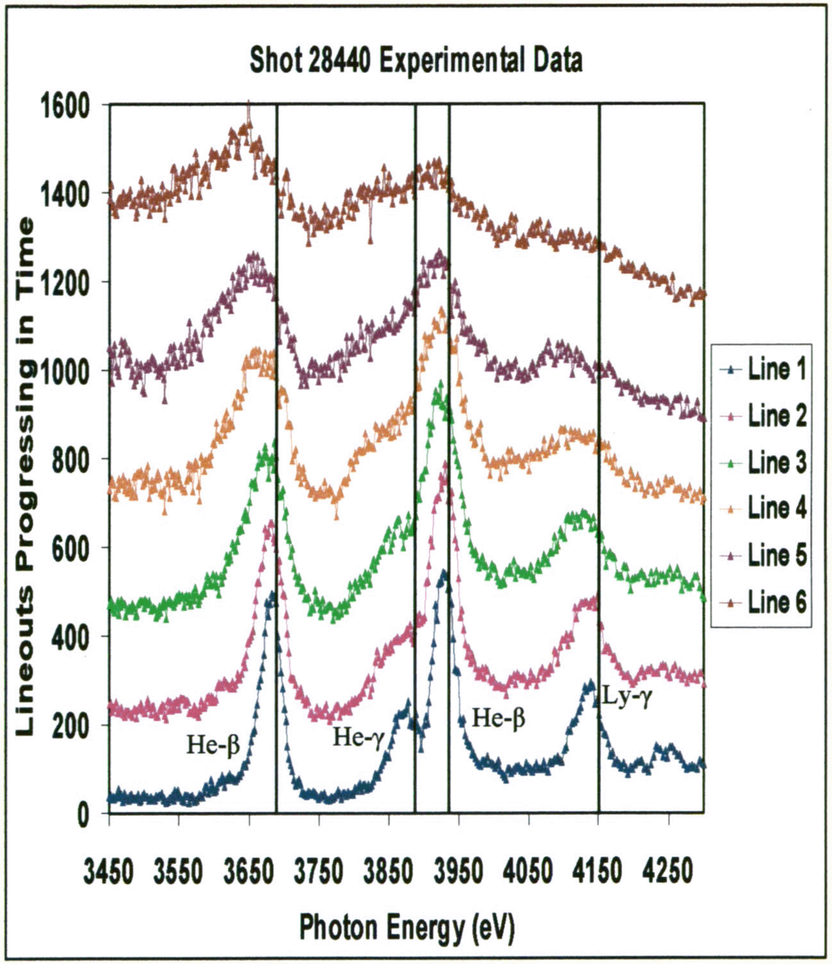
RAGE and HYADES Simulations of Electron Temperature for Omega Shot 28440





- HYADES, with its thermonuclear burn package, predicts a neutron yield of 1.28×10^{11}.

The experimental data from shot 28440 also shows a definite shifting of the lines as the implosion progresses.



- Again, using the theoretical predictions of how much the lines will shift, the density achieved in this implosion is around 3.5×10^{24} electrons/cc, or about 6 g/cc, before the spectral line become unobservable.
- The neutron yield from this shot was 1.47×10^{10}, and the bang time from the neutron data was 2.05 ns.
- Note the correlation between changes in the neutron yield and the electron density when this data is compared to that of shot 28435.
- One possible reason for the higher density on this shot is the slightly thinner shell (23.5 vs 26.5 microns).

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Summary and Conclusions

Line asymmetries and the corresponding shift of spectral lines due to the electron penetration of the radiator orbitals and the ion quadrupole contribution become more significant with increasing principal quantum number and increasing electron density.

- The mean field static shift due to electron penetration of the orbitals gives rise to an overall shift of the line to lower energy and a significant asymmetry near line center, but does not generate much red/blue far wing asymmetry.
- The ion quadrupole contribution results in a small blue shift of the spectral line and a small change in asymmetry near line center, but it gives rise to a significant red/blue wing asymmetry in the far wings of the line.
- Experimental data from recent spherical implosion experiments on OMEGA shows evidence of the mean field static shift and may also show the effects of level interactions between the Ar Lyman -γ, -δ, -ε lines and also the Ar He -γ, -δ lines.